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Final Report to the Office of Navel Research Department of the Navy 800 North Quincy Street Arlington, Virginia 22217

1982 GORDON RESEARCH CONFERENCE ON HIGH TEMPERATURE CHEMISTRY

> July 26-30, 1982 Tilton School Tilton, New Hampshire

Wayne L. Worrell
Conference Chairman
University of Pennsylvania

Philadelphia, Pa. 19104

Karl E. Spear Vice Chairman Pennsylvania State University University Fark, Pa. 16802 Alexander M. Chuickshank
Director, Gordon Research Conference
Department of Chemistry
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University of Rhode Island Kingston, Rhode Island 02381

Marie Daniel

August, 1982

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Final Report to the
Office of Navel Research
1982 Gordon Research Conference on
High Temperature Chemistry
July 26-30, 1982
Tilton School
Tilton, New Hampshire

Conference Chairman
Wayne L. Worrell
Materials Science Department/Kl
University of Pennsylvania
Philadelphia, Pa. 19104
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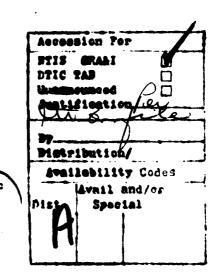
Vice Chairman Karl E. Spear Materials Research Lab. Pennsylvania State University University Park, PA 16802 (814) 865-1198

Background and Nature of Conference

The Gordon Research Conference on High Tempeerature Chemistry has been held biennially since 1960. As such, it is the only regularly scheduled international meeting where the interdisciplinary group comprising high temperature science can interact and discuss forefront issues of the day. Gordon Conference surveys of past participants have indicated this conference to be extremely helpful in the generation of new research ideas and contacts. The mix of foreign, local, academic, industrial and government participants is also a recognized hallmark of such meetings.

- The 1982 Conference had 17 invited talks in the areas of:

- Kinetics of Gas Phase Reactions;
- Surface Reactions;
- Chemical Vapor Transport
- Novel Investigations of Corrosion Reactions
- Thermodynamics of Liquids and Glasses;
- Solid State Electrochemistry;



- Muclear Reactor Accident Modeling and High Temperature Chemistry
- * Ab Initio Calculations of Molecular Structure and Propreties ...
- ° Spectroscopy of High Temperature Molecules ...

There were 38 invited poster presentations, which provided an additional forum for in-depth discussions of other active research topics in the field. The conference program and a list of invited poster papers are attachments A and B, respectively.

The conference had a total attendance of 105, including 20 from industrial laboratories, 30 from governmental laboratories, 40 from Universities and 15 from outside the U.S. Attachment C is a list of participants.

In accordance with Gordon Conference policy, no printed abstracts or papers were produced or distributed. The minutes of the conference business meeting, as prepared by the conference secretary, Dr. Clifford Myers, are appended as Attachment D.

Finances

A total of \$19,000 was available for disbursement by the conference chairman. Of this amount, the Gordon Research Conference provided \$7,500 (from conference fees), the Morgantown Energy Technology Center (NETC) contributed \$15,000, the Office of Navel Research (ONR) - \$3,000, the General Electric Company \$2,000, and IBM - \$7,500. These funds were used to offset the fixed conference fee (\$230) and/or travel expenses of key participants - primarily speakers and discussion leaders. Fifteen young scientists (postdoctoral and graduate students), whose attendance would otherwise not have been possible, were also supported by this fund. A budget summary of the OIR contribution is given in Attachment E.

Acknowledgment and Comments

Partial support of this conference by OLR is greatfully acknowledge. The 1982

Conference was pertinent to many of the navel research interests, particularly in the areas of corrosion reactions, solid-state electrichemisty, surface reactions and chemical vapor transport. We are confident that the free exchange of forefront information, so evident at this conference, will be benificial to exisiting and future ONR supported programs.

HIGH TEMPERATURE CHEMISTRY

July 26-30, 1982 Tilton School, Tilton, New Hampshire

Wayne L. Worrell, Chairman, and Karl E. Spear, VC

Monday, July 26

Kinetics of Gas Phase Reactions

"Kinetic Measurements of Free Calical and Gaseous Species"

"The Oxidation of Alkaline Earth Metal Vapors by N₂0"

Surface Reactions

"Relationships between Surface Structure and Catalytic Reactivity"

"Chlorine Reactions at Metal-Oxide Surfaces"

"Invited Poster Session on Recent Advances in High Temperature Chemistry'

Tuesday, July 27

Chemical Vapor Transport

'Complex Halide Vapors and their Significance in Vapor Transport

"Chemical Vapor Transport and Thermodynamic Analysis of Metal-Chalcogenide-Halide Systems"

Novel Investigations of Corrosion Reactions

"Hot Corrosion Reactions of Metals with Thin Salt Films"

"In-situ Raman Spectroscopic Characterization of Corrosion Reaction Products'

"Invited Poster Session on Recent Advances in High Temperature Chemistry"

Wednesday, July 28

Thermodynamics of Liquids and Glasses

"Thermodynamic Properties of Ordered Liquid Mextures"

D. L. Hildenbrand, Discussion Leader

C. E. Kolb Aerodyne Research, Inc.

P. J. Dagdigian John Hopkins University

G. M. Rosenblatt, Discussion Leader

D. Wayne Goodman Sandia National Laboratories

P. Nordine
Yale University

P. Gilles, Discussion Leader

H. Oye Norwegian Institute of Technology

H. Wiedemeier Rensselaer Polytechnic Institute

J. B. Vagner, Jr., Discussion Leader

R. A. Rapp Ohio State University

A. S. Nagelberg and J. C. Hamilton Sandia National Laboratories

L. Brewer, Discussion Leader

M. Blander Argonne National Laboratory

Wednesday, July 28, continued

"Structural Interpretations of the Thermodynamic Properties of Glasses and Crystals" Solid State Electrochemistry

'Transport Properties of Some Transition-Metal Oxides'

"HIgh Conductivity Solid Electrolytes'

"Invited Poster Session on Recent Advances in High Temperature Chemistry"

Thursday, July 29

Ab Initio Calculations of Molecular Structure and Properties Ab Initio Calculations of the Structure and Properties of Transition-Metal Gaseous Hydrides

"Ab Initio Calculations of the Properties of Molecules and "Atomic Clusters": Current Capabilities and Future Prospects

Nuclear Reactor Accident Modeling and High Temperature Chemistry

Specific Aspects

Friday, July 30

Spectroscopy of High Temperature Molecules

"Spectroscopy in Supersonic Polecular Beams: The Fluorescence of MaI

'Magnetic Circular Dichroism Spectra of Matrix Isolated High Temperature Molecules' A. Navrotsky Arizona State University

C B. Alcock, Discussion Leader

R. Dieckmann Universitat Hannover

G. C. Farrington, University of Pennsylvania

W. Weltner, Discussion Leader

H. F. Schaefer University of California, Berkeley

J. O. Arnold NASA-AMES Research Center

Overview D. D. Cubicciotti Electric Power Research Institute

Electric Power Research Institute

D. Olander, University of California M. Adamson, General Electric Vallecitos

R. Sallach, Sandia National Laboratories

P. Potter, AERE, Harwell

J. W. Hastie, Discussion Leader

D. H. Levy University of Chicago

M. Vala University of Florida

POSTER PAPERS FOR GORDOM RESEARCH COMFERENCE ON HIGH TEMPERATURE CHEMISTRY Tilton School, Tilton, New Hampshire July 26-30, 1982

Poster #	Presentation on Monday, on display Monday and Tuesday				
1	E. Fitzer and K. Brennfleck, University of Karlsruhe, West Germany "Superconducting $Mb(C,N)$ layers on carbon fibers by chemical vapor deposition and subsequent surface reactions"				
3	E.C. Beahm and O.L. Culberson, Oak Ridge National Laboratory 'Uncertainty analysis in thermodynamic calculations				
5	N.L. Saboungi, R.H. Yonco, Argonne National Laboratory and O. J. Kleppa, University of Chicago: "Enthalpy of mixing of liquid Rb-Au alloys"				
7	R.D. Brittain, D.L. Hildenbrand and K.H. Lau SRI International: "Thermodynamics of metal sulfate decomposition"				
9	J.G. Edwards, R. Haque, S. Kohirsagan, and A. Qusti, University of Toledo: "Discoveries about ternary sulfides through high-temperature vaporization studies				
11	R. Schiffman and P. Nordine, Yale University. "Containerless high temperature investigations by laser induced atomic fluorescence"				
13	R. Schoonmaker, Oberlin College: "Scattering of molecular beams from surfaces: dynamics of gas-surface interactions and the mechanism of condensation of cesium atoms and alkali halide molecules of NaCl (100)"				
15	D. M. Speros, General Flectric Co., Cleveland (Correlation between kinetic, crystallographic (surface structural) and thermodynamic quantities: Part I: Thermal dissociation of certain solids:				
17	R. W. Ohse, J.F. Babelot, J. Magill (European Institute for Transuranium Elements, Karlsruhe, W-Germany), C. Cercignani (Istituto di Matematica del Politecnico di Milano, Italy), A. Frezzotti (DIRES RICE-Alfa Romeo, Milano Italy), and J.P. Hiernaut, M. Hoch (University of Cincinnati): "High temperature vaporization of uranium oxide - consistency of mass spectrometric and depth measurement with thermodynamic calculations of the vapor pressure over U32 up to 5000 K"				
19	J. Hvistendahl (University of Tennessee), P. Klaeboe (University of Oslo, Norway) and E. Rytter, H.A. Øye (Norwegian Institute of Technology, Trondheim, Norway): "Emission IR spectra of chloroaluminate melts, improved technique for obtaining emission spectra of melts"				
21	Dean E. Peterson, Los Alamos National Laboratory: 'Thermodynamics of Actinide Intermetallics'				
23	J. M. Leitnaker, Oak Ridge Gaseous Diffusion Plant: "Thermodynamics of uranium-fluorine compounds"				

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Poster #	Presentation on TUESDAY, on display Bonday and Tuesday
2	E. Fitzer, J. Daimer and J. Schlichting, University of Karlsruhe, W-Germany "Kinetics and mechanism of the formation of self healing oxide layers on complex high temporature Si/Cr/Fi/Ta coatings and the attack under hot corrosion environments."
4	M.A. Frisch, IBC Thomas J. Vation Research Center: "Vaporization studies of non-congruent systems using modulated beam mass spectrometry
6	F. J. Kohl and J.L. Smiales, MASI Lewis Research Center, "Al ₂ 0 ₃ scale degradation by an applied electric field"
8	H. Tetenbaum Argonne National Laboratory 'High temperature vaporization behavior of the solid breeder blanket Li-0-H system'
10	A. II. Oner Yale University: "Transient studies of gasification Finetics by plasma emission spectroscopy"
12	S.A. Arthers, I.R. Beattie, T.R. Gilson, R.A. Gomme, S.N. Jenny, P.J. Jones, J.S. Ogden, J. Parkinson, and S. J. Williams, University of Southampton, England. Vibrational spectroscopy in the characterisation of high temperature vspours and melts with particular reference to alkali metal salts of oxoanions.
14	C.W. Draper, Western Electric Co., Princeton laser surface melting and alloying: a new method for producing metastable crystalline and amorphous metal surfaces.
16	V. B. Tare and J.B. Wagner, Jr. Arizona State University: Electrical Conduction in Two Phase Nickel Oxide-Nickel Sulfide Mixtures
18	M.G. Adamson and R.V. Caputi, General Electric Co., Vallecitos Nuclear Center: "Melting temperature determinations and urania-fission product systems with up to 5 components
20 (a)	J. Janitsch, K.L. Komarek and J. Likler, University of Vienna, Austria: "Calorimetric measurements on liquid gold-indium alloys
(b)	R. Krachler, P. Terzieff, H. Ipser and K.L. Komarek, University of Vienna, Austria. "Magnetic and thermolynamic properties of solid B'-AuMn"
22	P.D. Kleinschmidt and J.V. Gard, Los Alamos National Laboratory: "The role of f-electrons in actinide metal Londing"
24	C.E. Meyers, State University of New York. Binghamton. "Thermodynamic stabilities of transition metal phosphides and—related compounds

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Poster "	Presentation on WELWISTMY on discley Wednesday and Thursday				
1	H Saltsburg and Wellis the two versity of Rochester Observations of surface Omire non-during a hotorogeneous catalytic reaction				
3	E Halpern and I butat (Yalo University). D Grose (Harvard University) and L Douwon (University of Rochaster) "Thermionic emission from incandescent It during the surface decomposition of hydrocorbons and the exidation of adsorbed carbon				
5	R.J. Van Zee C Λ baumann S Λ Bhat and V Poltner, Jr., University of Florida Thigh temperature metal molecules				
7	K.E. Johnson University of Regina Canada 'Electrochemical promotion and following of high temperature reactions				
9	P.A. Montano and J. H. Magarathna, West Virginia University, "Electronic structure of bametallic molecules of FeCr. FeSn and FePt"				
11	J.W. Hastie, D.W. Bonnell and W.S. Horton, National Bureau of Standards: "Activity and phase equilibria models of high temperature liquid-solid-glass-gas systems"				
13	Z.K. Ismail, L. Fredin, R.W. Hauge, W.E. Billups and J.J. Margrave, Rice University "New Reactions of Metal Atoms"				
15	D.J. Frurip and H. Blander, Argonne National Laboratory "Production of sub-micron metal alloy and ceramic powders via laser pyrolysis"				
17	D.W. Bonnell and J.W. Hastie, Bational Bureau of Standards: "Fragmentation temperature dependence in electron impact ionization of molecular beams"				
19	M.W. Chase, Dow Chemical Company "JANAF thermochemical tables - reanalysis of the elements including sulfur and manganese				
21	P. Kofstad, University of Cslo, Morway "Defects and diffusion in metal deficient oxides				
23	J.E. Kingcade, Jr. and K.A. Gingerich. Texas A& University: "Gaseous transition metal compounds with carlon, silicon, germanium, and tin				
24	O.J. Kleppa, University of Chicago "Thermoclemistry of borides by high temperature solution calorimetry				

HIGH TEMPERATURE CHEMISTRY

K=Knowles
P=Pfeiffer
B=Beaumont
N=Mansion

Tilton School, Tilton, New Pampshire July 26-30, 1932

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Alcock, Charles Dept. of Metallurgy Materials S University of Toronto, Canada	120 wk cience	Casleton, Kent H. 336 wk USDOE/Norgantown Energy Technology Center P.O. Box 830, Collins Ferry Road	
		Porgantown, WV 26595	
Arnold, James O.	343 wic		
NASA-Ames Research Conter Hoffett	Field	Chase, Malcolm W.	7 b
CA 94035		The bw Chemical Co., 1707 Midland, MI 48640	Building
Bamberger, Carlos	104 ek		
Oak Ridge National Laboratory, P.	O. Pox X	Crumley Winfred	226 wk
Oak Ridge TN 37830		Georgia Institute of Techn North Ave., Chemistry	ology, 225
Beahm, Edward C.	115 ek	Atlanta GA 30332	
Oak Ridge National Laboratory, P.	O. Box X		
Bldg 4501, Oak Ridge, TN 37830		Cubicciotti, D.	6 Ь
		Electric Power Research In	
Beattie, Ian	344, wk	Box 10412, Palo Alto, CA	94303
The University, Southampton SO9 5	NH		
Hampshire, England 0703		Culberson, Oran L.	5 b
		Engr. Coor. & Anal. Sectio	
Blackburn, Paul E. and Joy		National Lab., Oak Ridge,	TN 37830
Argonne National Laboratory, 9700	S. Cass		
Argonne, IL 60439		Dagdigian, Paul J.	336 wk
		Johns Hopkins University,	Dept. of Chemistry
Blander, Milton	off campus	Baltimore, ND 21218	
Argonne National Lab., 9700 S. Ca	ss Ave.,		
Argonne, IL 60439		Davies, Peter	246 wk
		Arizona State University	
Bonnell, David	344 wk	Tempe, AZ 85281	
Mational Bureau of Standards			
4329/223 Div. 561, Washington, DO	20234	Dieckmann, R. and Christin	
		University of Hannover, In	
Betor, Jan P.	342 wk	Physical Chemistry, Hannov	er, W-Germany
University of Toledo			
		Draper Clifton	4 b
Bowker, Jeffrey	103 ek	Western Electric Engineeri	
Calgon Corp., P.O. Box 1346		F.O. Box 900, Frinceton, N	J 08540
Pittsburgh, PA 15230			
		Drowart, John	220 ek
Brennfleck, Karl	227 wk	Vrye Universitit Brussel,	Pleinlaan 2
Kaiserstrasse 12 7500 Karlsruhe		R-1050 Brussels, Belgium	
Provent Lee	18 b	Pinnada Hamis and Court	21 -
Brewer, Leo		Edwards, Jimmie and Carol	
Laurence Berkeley Lab, University		The University of Toledo,	
Dept. of Chemistry Berkeley, CA	9472"	Chemistry, Toledo, Ohio 4	2000
Brittain, Robert	337 vk	Faizi, Edgar	341 wk
SRI International, 333 Ravenswood		University of California,	
Henlo Park, CA 94025	* · * * * ,	Berkeley, CA 94720	sele of onemporty.
		Dermary, or 24160	
Carlson, K. Douglas	19-ь	Fontijn, Arthur	245 v/k
Argonne National Lab., Chemistry		Dept. of Chemistry, Rensse	
9700 S. Cass Ave., Argonne, IL &	0439	Inst. Troy, NY 12101	
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Goodman, David 244 wk GTE Sylvania, 100 endicott St., Danvers, MA 01923

Goodman, D. Wayne 245 wk. Sandia National Labs, Division 5114 Albuquerque, NM 87185

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Speros, Dimitri and Nel General Electric, Lighting Research Nela Park, Cleveland, OH 44112

Tare, Vasudeo Arizona State University, Ctr Solid State Science, Tempe, AZ 85287

High Temperature Chemistry -4-, 1982

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Ismail, Zakya 3 m Rice University, P.O. Box 1892 Houston, TX 77251

Olander, Donald 219 ek University of Berkeley, California Nuclear Engineering Berkeley, CA 94720

- 2. Every effort should be made to avoid scheduling the High Temperature Chemistry Conference on the same date as the conference on: Solid State Chemistry, Crystal amouth, Solid State Studies in Ceramics, tolecular Electronic Spectroscopy, Plasma chemistry.
- 3. The poster sessions should be continued with the following changes:
 - a) Display the posters at a time and place more convenient to the participants. For example, display the posters in the dining or snack bar area and hold the sessions from 5:30 6:30 P1.
 - b) Display only about 8 posters each day and do not leave the posters up for a second day.
 - c) Explore the possibility of allowing each poster presentor two minutes (one or two slides or transparencies) to present the title and a brief abstract of the poster at a time preceding each poster session.
- 4. Recommended topics for 1934, were presented and distributed to the conferees to assess their interest. (The list is attached to these minutes.

The Chariman express his thanks to Vice Chariman Karl Spear for his work in organizing and planning the poster sessions. Chairman—Elect Spear then expressed his thanks to Chairman Worrell for his efforts. He announced that the 1984 Gordon Research Conference on High Temperature Chemistry will be July 23-27, 1984, at Brewster Academy in Wolfeboro, N. H.

The meeting was adjorned at 12:25 Hi.

Respectfully submitted,

Clifford E. Myers, Secretary Gordón Research Conference on

High Temperature Chemistry

Tilton School Tilton, New Hampshire

July 26-30, 1902

Minutes at the Business Meeting

The business meeting of the conference was called to order by the Chairman, Wayne Worrell, following the morning session on Thursday, July 29, 1902, at 11:45 A.M. He reported that there were 105 conferees (15 were from outside the U.S.) of which 20 were from industry, 30 from government, and 40 from universities. The last included 15 "young" scientists (graduate students and post-doctoral associates).

The Chairman expressed appreciation to the speakers and participants. He noted that the discussions had been vigorous and of high quality. He also expressed appreciation for the service of the projectionist.

Following the tradition of the conference, it was moved, seconded and carried that Karl Spear, the 1982 Vice Chairman, be elected Chairman of the 1984 Conference.

The Vice Nominating Committee which had been named on the first day of the conference, consisted of:

Gerd Rosenblatt, (Chairman), Leo Brewer, K. Douglas Carlson, Daniel Cubicciotti, Paul Gilles, John Hastie, and Robert Thorn.

The committee's nominees for the post of Vice-Chairman for the 1984 conference were announced:

Donald Hildenbrand, SRI International Bruce Wagner, Arizona State University

A secret ballot resulted in the election of D. Hildenbrand.

The Chairman called on Bruce Wagner for the report of the Recommendations Committee. Committee members were:

Bruce Wagner (Chairman from Arizona State University), Clifton Draper (Western Electric Co.), Margaret Frisch (IEM), James Gole (Georgia Inst. Technol.), David Green (Argonne Natl. Lab.), Fred Kohl (NASA - Levis), Charles Kolb (Aerodyne Res. Inc.), Alexandra Novrotsky (Arizona State Univ.), and Dean Peterson (Los Alamos Natl. Lab.).

The Committee made the following recommendations:

 There should be a Gordon Research Conference on High temperature Chemistry in 1984.

TOPICS FOR 1984 CONFERENCE

PLEASE INDICATE YOUR PRIORITY OF INTEREST FOR EACH TOPIC: H (High), M (moderate), L (Low).
Return by noon Friday 7/30/82 or mail to Karl Spear.

- 1. Role of inorganic species in combustion
- 2. Negative ions of high temperature species
- 3. Analytical and diagnostic techniques: e.g. electrochemical sensors
- 4. Properties and measurements at temperatures above 3000K
- 5. Gas-solid reactions: experiments and theory
- 6. Resonance Raman spectroscopy
- 7. Microwave spectroscopy
- 8. Photoelectron spectroscopy
- 9. Supersonic beams
- 10. Hot stage microscopy
- 11. High pressure-high temperature systems
- 12. Alkali metal applications in fusion, fission, MHD
- 13. Intermetallics: formation in epi-layers
- 14. Liquid phase and molecular beam epitaxy
- 15. Vaporization: non-stoichiometry, incongruent vaporization, unusual gaseous species
- 16. Materials processing in low gravity
- 17. Clusters: formation, experiments, theory
- 18. Electron diffraction
- 19. Model studies on condensed phase equilibria
- 20. Molecular reaction dynamics: experiment and theory
- 21. Coal slags: spectroscopic and other studies
- 22. High temperature gaseous salutions
- 23. Overview of chemical transport
- 24. Rare earth solids and vapors
- 25. Model calculations on condensed phase dynamics
- 26. High temperature disposal of organic waste
- 27. Evaluation and compilation of thermophysical data
- 28. Geological and astro physical processes
- 29. New and innovative methods for metals production
- 30. Cohesive energies of high temperature solids

ATTACH ENT E

Budget Breakdown for OTR Contribution

1982 CRC on High Temperature Chemistry

A. Conference Fixed Fee (\$230) Support for 10 Participants

- 1. P. J. Dagdigian, The Johns Hopkins University
- 2. J. Edwards, University of Toledo
- 3. G. C. Farrington, University of Pennsylvania
- 4. R. Hauge, Rice University
- 5. D. Levy, University of Chicago
- 6. A. Navrotsky, Arizona State University
- 7. P. C. Nordine, Yale University
- K. E. Spear, Pennsylvania State University
- 9. !!. Vala, University of Florida
- 10. H. Wiedemeir, Rensselaer Polytechnic Institute

				\$2,300
в.	Don	nestic Travel Support		
	1.	L. Brewer, University of California		s 230
	2.	P. Gillis, University of Kansas		230
	3.	D. Levy, University of Chicago		\$\frac{250}{700}
			Total	\$3,000